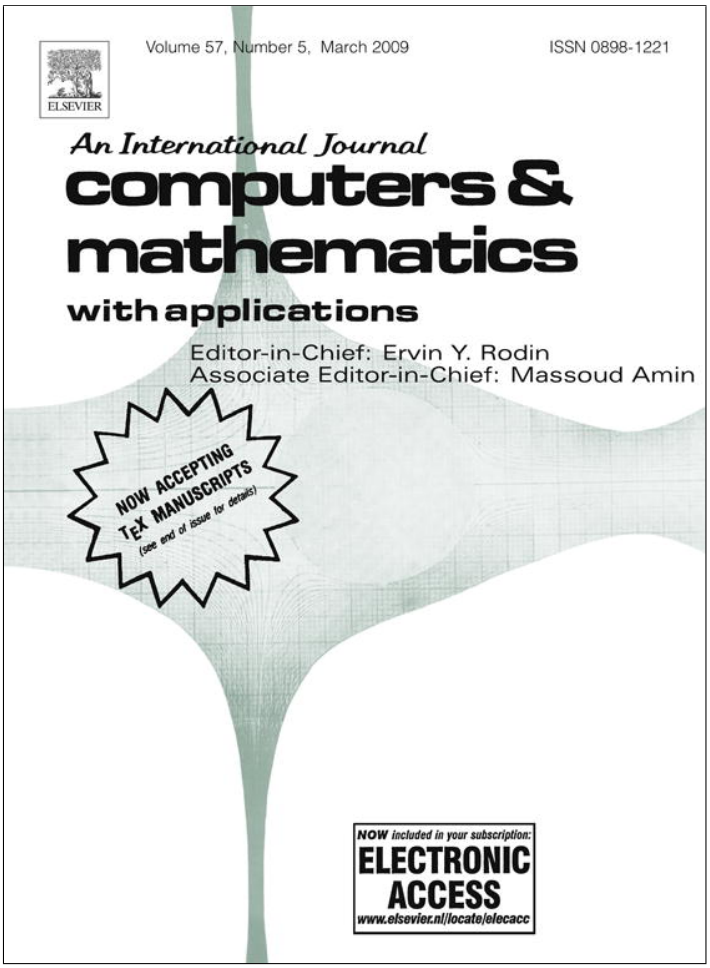

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The MWF method for kinetic equations system

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ABSTRACT

Many physical or biological phenomena deal with the dynamics of interacting entities. These class of phenomena are well described in physics, using a kinetic approach based on Boltzmann equation. A Generalized Kinetic theory has been proposed to extend this approach to biological scenarios. An analytical solution of Boltzmann equation can be found only in very simple cases, so numerical methods become extremely relevant. The particle method is a class of numerical methods used to find a numerical solution of Boltzmann equations. The MWF-method for kinetic equations was firstly proposed by S. Motta and J. Wick in 1992. Here, we show that the MWF-method can be extended to system of Boltzamm equations.

1. Introduction

Many physical or biological phenomena can be described by considering collections of interacting entities. These phenomena are well described, using a kinetic approach based on the Boltzmann equation, and extensively used in physics [1]. An extension of the Boltzmann equation to describe biological problems has been proposed [2–4]. In many biological problems, one needs to consider many different populations of interacting entities. In these cases, the problem is represented by a system of Boltzmann equations. The exact solution of a single Boltzmann equation is limited to simple and well known problems. System of coupled Boltzmann equations are obviously more difficult to solve analytically.

In some cases, one can analyze analytically reduced problems or asymptotic behaviors but, in most cases, one needs to resort to an approximate and numerical solution for the full problem. However, even an approximate solution of the Boltzmann equation is a hard problem, for which both analytical and numerical methods are continuously proposed [5–7]. Particle methods are in a class of numerical methods widely used for the Vlasov equation during the last three decades [8,9]. The extension of particle methods to the Boltzmann equation has been done mainly with two different strategies in treating the collision integral: a stochastic or a deterministic approach. Classical stochastic particle methods are based on the well known Montecarlo method [10], and simulate collision probabilities using stochastic events. New approaches on this line have been proposed in recent years [11–14]. Deterministic particle methods use particles as quadrature nodes for computing an approximate solution of collision integral. In most methods, particles are kept fixed in the velocity space and the evolution is reflected in changing their weights in time. This is a well established technique, and it is used in many applications [14–16].

In the framework of deterministic particle methods, a different approach was presented by Motta and Wick [17]. A new formulation of the method, oriented for implementation purposes was later presented by Motta [18,19]. Particles are allowed to move in the velocity space, while the particle weight is kept constant. The idea of the method (hereafter referred simply as MWF-method) is to write the equation in divergence form and formally to transform the problem into a collisionless one.

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This can be done by introducing a flux equivalent for the inhomogeneity and by computing, at each time step, the *collision induced force term* for the *collisionless* problem.

In the first paper, the method was numerically tested with model equations. Then, the relevant quantities of the method for semiconductor kernels in 2D and 3D were derived by Barone and Motta [20,21]. The method was applied to the classical test case of a semiconductor $N^+N^-N^+$ structure, showing that the method can be implemented on a parallel computer [22]. Comparison with other particle methods was presented by Wick [23].

In the present paper, we take the matter again, using the latter formulation [18] and we show the extension of the method to a system of coupled Boltzmann equations. The general approach is then applied to a linear collision kernel to test the numerical solution vs an exact solution.

The plan of the paper is the following: in Section 2 we write the system of kinetic equations to solve; in Section 3 we extend the MWF method for a system of kinetic equations and show that the solution is gauge invariant; in Section 4 we consider the case of a linear collision kernel, and we write the exact solution of this problem which we then compare with numerical solution obtained by the MWF method. Finally, in Section 5, we draw some conclusions and plans for further investigation.

2. The Kinetic equations system

Let $\mathbf{f} = (f_1, f_2, \ldots, f_n)^{\mathrm{T}} \in \mathbb{R}^{n\times 1}$ be a vector function whose components

$$f_i(x, v, t) : \Omega_x \times \Omega_v \times [0, \infty] \to \mathbb{R}, \quad i = 1, 2, \ldots, n$$

are scalar functions of $x \in \Omega_x \subset \mathbb{R}^3$, $v \in \Omega_v \subset \mathbb{R}^3$ and $t \geq 0$. Here, $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ denotes a typical point in space, $v = (v_1, v_2, x_3) \in \mathbb{R}^3$ denotes a typical point in velocity and $t \geq 0$ denotes a typical time.

A kinetic equations system (KES) is the following system of first-order, semi-linear partial differential equations

$$\partial_t \mathbf{f} + \mathbf{div}_{(x,v)}(\mathbf{f}(\mathbf{u}, \mathbf{F})) = \mathbf{Q}(\mathbf{f}), \tag{1}$$

involving the unknown vector function $\mathbf{f} = (f_1, f_2, \ldots, f_n)^{\mathrm{T}} \in \mathbb{R}^{n\times 1}$, where

$$\mathbf{u}(v) = (u_1(v), u_2(v), \ldots, u_n(v)) : \Omega_v \to \mathbb{R}^n, \tag{2}$$

$$\mathbf{F}(x, t) = (F_1(x, t), F_2(x, t), \ldots, F_n(x, t)) : \Omega_v \times [0, \infty] \to \mathbb{R}^n, \tag{3}$$

$$\mathbf{Q}(\mathbf{f}) = (Q_1(\mathbf{f}), Q_2(\mathbf{f}), \ldots, Q_n(\mathbf{f})) : \mathbb{R}^n \to \mathbb{R}^n, \tag{4}$$

are given vector fields and

$$\mathbf{div}_{(x,v)}(\mathbf{f}(\mathbf{u}, \mathbf{F})) = \begin{pmatrix} \mathrm{div}_x(f_1u_1) + \mathrm{div}_v(f_1F_1) \\ \mathrm{div}_x(f_2u_2) + \mathrm{div}_v(f_2F_2) \\ \vdots \\ \mathrm{div}_x(f_nu_n) + \mathrm{div}_v(f_nF_n) \end{pmatrix}.$$

The inhomogeneity $\mathbf{Q}(\mathbf{f})$ is usually a collision integral which describes short range interactions.

Here, we suppose that the system comprises the same number n of scalar equations as unknowns f_i, $i = 1, 2, \ldots, n$.

The (KES) is solved if we find all $\mathbf{f}$ verifying (1), possibly only among those functions satisfying certain auxiliary boundary conditions (classical solution). By finding the solution means, ideally, obtaining explicit solutions, or, failing that, deducing the existence and other properties of solutions. There is no general theory, to the best of our knowledge, known concerning the solvability of the (KES). Such a theory is extremely unlikely to exist, given the rich variety of physical and probabilistic phenomena which can be modeled by (KES).

Let $\Omega = \Omega_x \times \Omega_v$ be the cartesian product of Ω_x and Ω_v. We look for a solution of (1) in the following space functions:

$$\mathcal{M}(\Omega) = \left\{ \mathbf{f} = (f_1, f_2, \ldots, f_n) : \Omega \times [0, \infty] \to \mathbb{R}^n : \quad f_i \geq 0, \int_\Omega f_i(x, v, t)\, \mathrm{d}x\, \mathrm{d}v = 1 \right\} \tag{5}$$

under the conservation hypothesis

$$\int_{\Omega_v} Q_i(\mathbf{f})\, \mathrm{d}v = 0, \quad i = 1, 2, \ldots, n. \tag{6}$$

To the system (1) we associate an initial condition $\mathbf{f}_0(x, v) = (f_1^0, f_2^0, \ldots, f_n^0) \in \mathcal{M}(\Omega)$, such that

$$\mathbf{f}(x, v, 0) = \mathbf{f}_0(x, v).$$

The latter choice and the conservation property (6) guarantees that the solution $\mathbf{f}$ belong to the space $\mathcal{M}(\Omega)$ for all times. Then $\mathbf{f}(\cdot, t)$ can be interpreted as the density of probability measure $\mu(t)$.

3. The extension of the MWF method

The MWF method consists in rewriting the (KES) (1) in a conservation law in divergence form, redefining the collisions as a flux (CRF). To do that, one rewrites the collision term $\mathbf{Q}(\mathbf{f})$ as divergence of a flux $\mathbf{\Psi}$, and formally transform the problem in a collisionless one.

Let $\mathbf{\Psi} = [\psi_j^i] \in \mathbb{R}^{n\times 3}$ be the following matrix

$$\mathbf{\Psi} = \begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \\ \vdots \\ \psi^{(n)} \end{pmatrix} = \begin{pmatrix} \psi_1^{(1)} & \psi_2^{(1)} & \psi_3^{(1)} \\ \psi_1^{(2)} & \psi_2^{(2)} & \psi_3^{(2)} \\ \vdots & \vdots & \vdots \\ \psi_1^{(n)} & \psi_2^{(n)} & \psi_3^{(n)} \end{pmatrix}$$

such that

$$\operatorname{div}_v \psi^{(i)} = -Q_i(\mathbf{f}), \quad i = 1, 2, \ldots, n \tag{7}$$

$$\psi^{(i)} \cdot \mathbf{n}_{\Omega_v} = 0, \quad v \in \Omega_v. \tag{8}$$

The last conditions mean that $\mathbf{Q}(\mathbf{f})$ is expressed as a flux $\mathbf{\Psi}$. Moreover the boundary condition guarantees the conservative property of the system.

Now, we look for a matrix $\mathbf{G} = [g_j^{(i)}] \in \mathbb{R}^{n\times 3}$, such that

$$\mathbf{\Psi} = \mathbf{f}\,\mathbf{e}_1\,\mathbf{G},$$

where $\mathbf{e}_1 = (1, 0, \ldots, 0)$ is the first element of the canonical basic of $\mathbb{R}^n$. The last decomposition allow us to write

$$\mathbf{\Psi} = \begin{pmatrix} f_1 g_1^{(1)} & f_1 g_2^{(1)} & f_1 g_3^{(1)} \\ f_2 g_1^{(2)} & f_2 g_2^{(2)} & f_2 g_3^{(2)} \\ \vdots & \vdots & \vdots \\ f_n g_1^{(n)} & f_n g_2^{(n)} & f_n g_3^{(n)} \end{pmatrix}$$

and in a compact way as $\mathbf{\Psi} = [\psi_j^{(i)}] = [f_i\, g_j^{(i)}]$ for $i = 1, 2, \ldots, n$ and $j = 1, 2, 3$.

Thus, $\mathbf{G}$ is a velocity matrix associated with $\mathbf{f}$, whose physical dimensions are those of a force field. Taking the above considerations into account, the (KES) defined in (1) thus read

$$\partial_t \mathbf{f} + \mathbf{div}_{(x,v)}(\mathbf{f}\,(\mathbf{u}, \mathbf{F} + \mathbf{e}_1\mathbf{G})) = 0. \tag{9}$$

This system is formally identical to a Vaslov equation. Since the element of $\mathbf{G}$ are added to the given vector field, only the computation of $\mathbf{G}$ is needed.

3.1. The computation of the force matrix $\mathbf{G}$

Since we are interested in treating the collision term, we restrict our attention to the spatially homogeneous problem, i.e. $\mathbf{f} = \mathbf{f}(v, t)$ and $\mathbf{G} = \mathbf{G}(v, t)$. Let $\mu(B)$ and $\nu(B)$ be the following measures

$$\mu(B) = \int_B \psi_j^{(i)}\, \mathrm{d}v,$$

$$\nu(B) = \int_B g_j^{(i)}\, \mathrm{d}v.$$

Since the measure μ is then absolutely continuous with respect to ν, the force-matrix $\mathbf{G}$ can be computed, interpreting each f_i as the Radon–Nikodyn derivative of the μ with respect to ν. Integrating in Borel sets $B \subset \Omega_v$, we obtain for each component

$$\int_B f_i\, g_j^{(i)}\, \mathrm{d}v = \int_B \psi_j^{(i)}\, \mathrm{d}v, \tag{10}$$

for $i = 1, 2, \ldots, n$ and $j = 1, 2, 3$.

To compute the components of the induced force on each particle $g_{j,r}^{(i)}$ ($j = 1, 2, 3$, $r = 1, 2, \ldots, N$, $i = 1, 2, \ldots, n$). Fixed i, we need $3N$ relations that can be obtained by integrating (10) along the subset of Ω_v that constitutes a partition of Ω_v.

Suppose that in the chosen coordinate system, the momentum space Ω_v can be represented as a Cartesian product of three intervals

$$\Omega_v = \prod_{i=1}^{3} [\alpha_i, \beta_i],$$

with α_i and β_i can be eventually $-\infty$ and ∞ respectively. As a partition of Ω_v, we consider three different partitions of Ω_v, one for each component $g_{j,r}^{(i)}$ for $j = 1, 2, 3$. To compute $g_{j,r}^{(i)}$, we divide the interval $[\alpha_j, \beta_j]$ in the following way

$$\Omega_v = \bigcup_{r=1}^{N} I(k_j^{r-1}, k_j^{r+1}) = \bigcup_{r=1}^{N} I_j^r,$$

where $I(k_j^{r-1}, k_j^{r+1})$ is defined as

$$I(k_j^{r-1}, k_j^{r+1}) = \{v \in \Omega_v : k_j^{r-1} \le v_j \le k_j^{r+1}\},$$

and $k_j^0 = \alpha_j$, $k_j^{N+1} = \beta_j$. Each set I_j^r is the portion of Ω_v delimited by the planes $v_j = k_j^{r-1}$ and $v_j = k_j^{r+1}$.

We also suppose, in the previous definition, that particles are ordered according to the j-coordinate ordering. Moreover the sets I_j^r, $r = 2, \ldots, N-1$, contains only three particles, one on each boundary and the sets I_j^1, I_j^N contain two particles.

Integrating (10) on each I_j^r

$$\int_{I_j^r} f_i g_j^{(i)} \, \mathrm{d}v = \int_{I_j^r} \psi_j^{(i)} \, \mathrm{d}v, \tag{11}$$

we get the $3Nn$ relations. We define the right hand side of (11) as

$$\Psi_{j,r}^{(i)} = \int_{I_j^r} \psi_j^{(i)} \, \mathrm{d}v$$

and

$$\Psi_j^{(i)} = \begin{pmatrix} \Psi_{j,1}^{(i)} \\ \Psi_{j,2}^{(i)} \\ \vdots \\ \Psi_{j,N}^{(i)} \end{pmatrix}$$

for $j = 1, 2, 3$.

The left hand side of (11) can be evaluated, by using a suitable integration formula in each interval. If, for instance, we use a Simpson's rule, we get three linear system of order N for each $i = 1, 2, \ldots, n$ in the unknown $g_{j,r}^{(i)}$

$$\mathcal{A}^i \, \Gamma_j^{(i)} = \Psi_j^{(i)} \tag{12}$$

for $i = 1, 2, \ldots, n, j = 1, 2, 3, r = 1, 2, \ldots, N$, where $\Gamma_j^{(i)} = (g_{j,1}^{(i)}, \ldots, g_{j,N}^{(i)})^{\mathrm{T}} \in \mathbb{R}^{N\times 1}$ and $\mathcal{A}^i \in \mathbb{R}^{N\times N}$ is a fixed matrix, depending on the chosen quadrature formula. To solve these linear systems, it is necessary to compute the terms $\Psi_{j,r}^{(i)}$ as function of the collision kernel $\mathbf{Q}(\mathbf{f})$. Moreover, one should be guaranteed that the matrix $\mathcal{A}^i$ is not singular, which is the case when one choose Simpson's rule.

Let γ_j be a constant $\alpha_j \le \gamma_j \le \beta_j$, we consider the portion of Ω_v delimited by the planes $v_j = \alpha_j$ and $v_j = \gamma_j$

$$I(\alpha_j, \gamma_j) = \{v \in \Omega_v : \alpha_j \le v_j \le \gamma_j\}.$$

Let $F_j^{(i)}(\gamma_j)$ be the integral function

$$F_j^{(i)}(\gamma_j) = \int_{I(\alpha_j,\gamma_j)} \psi_j^{(i)}(v) \, \mathrm{d}v.$$

Proposition 3.1. *For $\alpha_j \le \gamma_j \le \beta_j$*

$$F_j^{(i)}(\gamma_j) = -\int_{I(\alpha_j,\gamma_j)} \left(\int_{\alpha_j}^{v_j} Q_i(\mathbf{f}) \, \mathrm{d}v_j' \right) \mathrm{d}v.$$

Proof. Let $\Gamma(\gamma_j)$ be the set of the vectors in Ω_v which belong to the plane $v_j = \gamma_j$

$$\Gamma(\gamma_j) = \{v \in \Omega_v : v_j = \gamma_j\} = \prod_{k=1}^{j-1} [\alpha_k, \beta_k] \times \gamma_j \times \prod_{k=j+1}^{3} [\alpha_k, \beta_k].$$

This surface does not belong to the $\partial\Omega_v$, and it has the outward normal vector along the axis v_j and versus along increasing v_j, i.e.

$$\mathbf{n}_{\Gamma(\gamma_j)} \cdot \hat{v}_j = 1.$$

Let $\overline{\gamma_j}$ be such that $\alpha_j \leq \overline{\gamma_j} \leq \gamma_j$,

$$-\int_{I(\alpha_j,\overline{\gamma_j})} Q_i(\mathbf{f})\,\mathrm{d}v = \int_{I(\alpha_j,\overline{\gamma_j})} \operatorname{div}\psi^{(i)}\,\mathrm{d}v.$$

By applying the Gauss divergence theorem, we have

$$\int_{I(\alpha_j,\overline{\gamma_j})} \operatorname{div}\psi^{(i)}\,\mathrm{d}v = \int_{\Gamma(\overline{\gamma_j})} \psi_j^{(i)}(\ldots, v_j = \overline{\gamma_j}, \ldots)\,\mathrm{d}S_j,$$

where $\mathrm{d}S_j$ is the surface element on the plane $v_j = \overline{\gamma_j}$. Since

$$\int_{\Gamma(\overline{\gamma_j})} \psi_j^{(i)}(v_{j-1}, \overline{\gamma_j}, v_{j+1})\,\mathrm{d}S_j = \prod_{k\neq j}^{1,2,3} \int_{\alpha_k}^{\beta_k} \psi_j^{(i)}(\ldots, v_j = \overline{\gamma_j}, \ldots) \prod_{i\neq j}^{1,2,3} \mathrm{d}v_i.$$

We have obtained that

$$-\int_{I(\alpha_j,\overline{\gamma_j})} Q_i(\mathbf{f})\,\mathrm{d}v = \prod_{k\neq j}^{1,2,3} \int_{\alpha_k}^{\beta_k} \psi_j^{(i)}(\ldots, v_j = \overline{\gamma_j}, \ldots) \prod_{i\neq j}^{1,2,3} \mathrm{d}v_i.$$

Since the last equality holds for all $\alpha_j \leq \overline{\gamma_j} \leq \gamma_j$, we can change the name of the variable $\overline{\gamma_j}$ into v_j, then

$$-\int_{I(\alpha_j,v_j)} Q_i(\mathbf{f})\,\mathrm{d}v' = \prod_{k\neq j}^{1,2,3} \int_{\alpha_k}^{\beta_k} \psi_j^{(i)}(v_{j-1}, v_j, v_{j+1}) \prod_{i\neq j}^{1,2,3} \mathrm{d}v_i.$$

The last integral is a function of v_j, now integrating in $[\alpha_j, \gamma_j]$, we obtain for the right hand side

$$\int_{\alpha_j}^{\gamma_j} \left[\prod_{k\neq j}^{1,2,3} \int_{\alpha_k}^{\beta_k} \psi_j^{(i)}(v_{j-1}, v_j, v_{j+1})\,\mathrm{d}v_{j-1}\,\mathrm{d}v_{j+1}\right] \mathrm{d}v_j \equiv F_j^{(i)}(\gamma_j)$$

and for the left hand side, we have

$$-\int_{\alpha_j}^{\gamma_j} \left(\int_{I(\alpha_j,v_j)} Q_i(\mathbf{f})\,\mathrm{d}v'\right) \mathrm{d}v_j = -\int_{I(\alpha_j,\gamma_j)} \left(\int_{\alpha_j}^{v_j} Q_i(\mathbf{f})\,\mathrm{d}v_j'\right) \mathrm{d}v. \quad \square$$

Proposition 3.2. *The terms $\Psi_{j,r}^{(i)}$ are given by*

$$\Psi_{j,r}^{(i)} = F_j^{(i)}(k_j^{r+1}) - F_j^{(i)}(k_j^{r-1}).$$

Proof. By the last proposition we have:

$$\Psi_{j,r}^{(i)} = \int_{I(k_j^{r-1},k_j^{r+1})} \psi_j^{(i)}\,\mathrm{d}v = -\int_{I(k_j^{r-1},k_j^{r+1})} \left(\int_{\alpha_j}^{v_j} Q_i(\mathbf{f})\,\mathrm{d}v_j'\right) \mathrm{d}v.$$

Since $I[k_j^{r-1}, k_j^{r+1}] = I[\alpha_j, k_j^{r+1}] \setminus I[\alpha_j, k_j^{r-1}]$ the last integral can be written as

$$\Psi_{j,r}^{(i)} = -\int_{I[\alpha_j,k_j^{r+1}]} \left(\int_{\alpha_j}^{v_j} Q_i(\mathbf{f})\,\mathrm{d}v_j'\right) \mathrm{d}v + \int_{I[\alpha_j,k_j^{r-1}]} \left(\int_{\alpha_j}^{v_j} Q_i(\mathbf{f})\,\mathrm{d}v_j'\right) \mathrm{d}v$$

and we have the proof by definition of the function $F_j^{(i)}$. $\square$

Remark 3.3. The definition of $\psi^{(i)}$ for $i = 1, 2, \ldots, n$ is not unique. Indeed, if $\psi^{(i)}$ satisfy (7), for every vector field $\chi^{(i)}$, the vector field

$$\varphi^{(i)} = \psi^{(i)} + \nabla \times \chi^{(i)},$$

will satisfy (7) as well. This is a trivial consequence of the fact that $\nabla \cdot (\nabla \times \chi^{(i)}) = 0$.

Nevertheless, the results obtained using the MWF method do not depend on the choice of a particular gauge in definition (7).

Theorem 3.4 (*The Gauge Invariance*). *The results of the MWF method do not depend on the choice of the matrix* $\mathbf{\Psi}$*, satisfying* (7).

Proof. We need only to show that $\Psi_{j,r}^{(i)}$ does not depend on the gauge $\mathbf{P}$. Since

$$\Psi_{j,r}^{(i)} = \int_{I(k_j^{r-1},k_j^{r+1})} \psi_j^{(i)}\,\mathrm{d}v \tag{13}$$

$$= \int_{I(\alpha_i,k_j^{r+1})} \psi_j^{(i)}\,\mathrm{d}v - \int_{I(\alpha_i,k_j^{r-1})} \psi_j^{(i)}\,\mathrm{d}v \tag{14}$$

$$= \int_{\alpha_i}^{k_j^{r+1}} \int_{\Gamma(v_j')} \psi_j^{(i)}(v_j')\,\mathrm{d}S_j\,\mathrm{d}v_j' - \int_{\alpha_i}^{k_j^{r-1}} \int_{\Gamma(v_j')} \psi_j^{(i)}(v_j')\,\mathrm{d}S_j\,\mathrm{d}v_j' \tag{15}$$

$$= \int_{\alpha_i}^{k_j^{r+1}} \int_{I(\alpha_j,k_j')} \operatorname{div}\psi^{(i)}\,\mathrm{d}v\,\mathrm{d}v_j' - \int_{\alpha_i}^{k_j^{r-1}} \int_{I(\alpha_j,k_j')} \operatorname{div}\psi^{(i)}\,\mathrm{d}v\,\mathrm{d}v_j' \tag{16}$$

$$= \int_{k_j^{r-1}}^{k_j^{r+1}} \operatorname{div}\psi^{(i)}\,\mathrm{d}v\,\mathrm{d}v_j', \tag{17}$$

where in the last equality it was used the Gauss divergence theorem. □

4. The linear collisional terme case

In this section, we consider $\mathbf{F} \equiv 0$, $\mathbf{u} \equiv 0$ and a linear collisional kernel $\mathbf{Q}(\mathbf{f})$. Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be a matrix whose elements are a_{ij}. The kernel has the following form

$$\mathbf{Q}(\mathbf{f}) = \mathbf{A}\,\mathbf{f}.$$

The (KES) considered is

$$\partial_t \mathbf{f} = \mathbf{A}\,\mathbf{f}. \tag{18}$$

Definition 4.1. A matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is called MWF-conservative if the sum of the elements of every rows is equal zero, i.e.

$$\sum_{j=1}^{n} a_{ij} = 0, \quad i = 1, 2, \ldots, n.$$

Lemma 4.2. *A MWF-conservative matrix is singular.*

Proof. The endomorphism f from $\mathbb{R}^n$ to $\mathbb{R}^n$, which has the matrix $\mathbf{A}$ associated with the canonical base of $\mathbb{R}^n$ is not an isomorphism, since the vectors $(1, 1, \ldots, 1) \in \mathbb{R}^n$ belong to the kernel of f. □

Proposition 4.3. *The matrix* $\mathbf{A}$ *of system* (18) *is a MWF-conservative matrix.*

Proof.

$$\mathbf{0} = \partial_t \int_{\Omega_v} \mathbf{f}\,\mathrm{d}v = \int_{\Omega_v} \mathbf{A}\,\mathbf{f}\,\mathrm{d}v = \mathbf{A}\,\mathbf{I}. \quad \square$$

It is interesting to observe that, from a point of view of the solutions, this problem can be considered as a system of ordinary differential equations where the constants are function of the velocity v. This is a consequence of the fact that there are only partial derivatives with respect the time. In this context the exponential matrix of $\mathbf{A}$

$$\mathrm{e}^{\mathbf{A}} = \sum_{k=0}^{+\infty} \frac{\mathbf{A}^k}{k!},$$

is a solution matrix. This fact allow us to prove the following result.

Theorem 4.4. *Let $\mathbf{f}^0(v) \in C^1[\Omega_v]$, then there exists one and only one solution $\mathbf{f}$ of the following Cauchy problem*

$$\begin{cases} \partial_t \mathbf{f} = \mathbf{A}\,\mathbf{f}, \\ \mathbf{f}(0, v) = \mathbf{f}^0(v). \end{cases} \tag{19}$$

Proof. Let $e^{t\mathbf{A}}$ be the solution exponential matrix. For every $g(x, v) \in \mathbb{R}^n$

$$\widetilde{\mathbf{f}} = e^{t\mathbf{A}}\, g(x, v),$$

is solution of $\partial_t \mathbf{f} = \mathbf{A}\,\mathbf{f}$. Indeed

$$\partial_t \widetilde{\mathbf{f}} = \mathbf{A}\, e^{t\mathbf{A}}\, g(x, v) = \mathbf{A}\,\widetilde{\mathbf{f}}.$$

The above considerations allow us to say that the solution of (19) is

$$\mathbf{f} = e^{t\mathbf{A}}\,\mathbf{f}^0(v).$$

Now we prove that the solution is unique. If $\widetilde{\mathbf{f}}$ and $\widehat{\mathbf{f}}$ are two distinct solutions of (19), the function $\mathbf{h} = \widetilde{\mathbf{f}} - \widehat{\mathbf{f}}$ satisfies

$$\begin{cases} \partial_t \mathbf{h} = \mathbf{A}\, h, \\ \mathbf{h}(0, v) = 0. \end{cases}$$

The solution of the above problem is $\mathbf{h} \equiv 0$. This implies the proof. □

The case $n = 2$. Consider the problem

$$\begin{cases} \partial_t f_1 = -\alpha f_1 + \alpha f_2, \\ \partial_t f_1 = \beta f_1 - \beta f_2, \end{cases}$$

with initial condition

$$f_1(v, 0) = f_1^0(v), \qquad f_2(v, 0) = f_2^0(v).$$

In this case

$$\mathbf{Q}(f_1, f_2) = \begin{pmatrix} Q_1(f_1, f_2) \\ Q_2(f_1, f_2) \end{pmatrix} = \begin{pmatrix} -\alpha(f_1 - f_2) \\ \beta(f_1 - f_2) \end{pmatrix}.$$

The exponential matrix and the vector solution are respectively

$$e^{t\mathbf{A}} = \begin{pmatrix} \dfrac{b}{a+b} + \dfrac{a}{a+b}\, e^{-(\alpha+\beta)t} & \dfrac{a}{a+b}\,(1 - e^{-(\alpha+\beta)t}) \\ \dfrac{b}{a+b}\,(1 - e^{-(\alpha+\beta)t}) & \dfrac{a}{a+b} + \dfrac{b}{a+b}\, e^{-(\alpha+\beta)t} \end{pmatrix}$$

$$\begin{cases} f_1(v, t) = \dfrac{\beta}{\alpha+\beta} f_1^0(v) + \dfrac{\alpha}{\alpha+\beta} f_2^0(v) + \dfrac{\alpha}{\alpha+\beta}\,(f_1^0(v) - f_2^0(v))\, e^{-(\alpha+\beta)t} \\ f_2(v, t) = \dfrac{\alpha}{\alpha+\beta} f_1^0(v) + \dfrac{\alpha}{\alpha+\beta} f_2^0(v) - \dfrac{\beta}{\alpha+\beta}\,(f_1^0(v) - f_2^0(v))\, e^{-(\alpha+\beta)t}. \end{cases}$$

4.1. Numerical example

In this section, we give a numerical example to estimate the accuracy of the method. It is well known that numerical accuracy depends on many parameters, also including the hardware platform; however an extensive analysis of numerical accuracy of the method is not in the aim of the present paper. In the following, we will simply compare a numerical solution versus an exact one, to give an estimate of the numerical errors. Exact solutions of Boltzmann equations are very rare, and usually restricted to the simple case of relaxation problems. Here we consider a relaxation problem in the case $n = 2$ with

$$\mathbf{f} = (f_1(x, y, t), f_2(x, y, t)),$$

where $(x, y) \in [0, 1] \times [0, 1]$, $(\alpha, \beta) = (1, 1)$ and initial conditions $f_1(x, y, 0) = f_1^0(x, y)$, $f_2(x, y, 0) = f_2^0(x, y)$. The exact solution thus read

$$f_1(x, y, t) = \frac{1}{2}\,(f_1^0(x, y) + f_2^0(x, y)) + \frac{1}{2}\,(f_1^0(x, y) - f_2^0(x, y))\, e^{-2t},$$

$$f_2(x, y, t) = \frac{1}{2}\,(f_1^0(x, y) + f_2^0(x, y)) - \frac{1}{2}\,(f_1^0(x, y) - f_2^0(x, y))\, e^{-2t}.$$

Table 1
Errors in the l^2-norm for f_1 numerical moments

Error	f_1
$\mathcal{E}_x^1$	7.07×10^{-14}
$\mathcal{E}_y^1$	2.00×10^{-4}
$\mathcal{E}_{xx}^1$	2.47×10^{-2}
$\mathcal{E}_{yy}^1$	1.22×10^{-2}
$\mathcal{E}_{xy}^1$	6.23×10^{-4}

As initial conditions, we choose $f_1^0(x, y), f_2^0(x, y) \in \mathcal{M}(\Omega)$, such that

$$f_1^0(x, y) = f_1^0(x) = 1 - \cos 2\pi x$$
$$f_2^0(x, y) = f_2^0(y) = 1 - \cos 2\pi y.$$

By using the Proposition 3.2, we have

$$\Psi_{1,r}^{(1)} = \frac{e^{-2t}}{4\pi^2}(\cos 2\pi x_1^r - 1), \qquad \Psi_{2,r}^{(1)} = \frac{e^{-2t}}{4\pi^2}(1 - \cos 2\pi y_1^r)$$

and

$$\Psi_{1,r}^{(2)} = -\frac{e^{-2t}}{4\pi^2}(\cos 2\pi x_2^r - 1), \qquad \Psi_{2,r}^{(2)} = -\frac{e^{-2t}}{4\pi^2}(1 - \cos 2\pi y_1^r).$$

The comparison of the numerical solution versus the exact solution is obtained via the first and the second moments. From the exact solution f_i, $i = 1, 2$, one can easily compute all the first and the second moments:

$$\mu_x^i(t) = \int_0^1 \int_0^1 x f_i(x, y, t)\mathrm{d}x\mathrm{d}y = \frac{1}{2},$$
$$\mu_y^i(t) = \int_0^1 \int_0^1 y f_i(x, y, t)\mathrm{d}x\mathrm{d}y = \frac{1}{2},$$
$$\mu_{xx}^i(t) = \int_0^1 \int_0^1 x^2 f_i(x, y, t)\mathrm{d}x\mathrm{d}y = \frac{1}{3} + \frac{1 + e^{-2t}}{4\pi^2},$$
$$\mu_{yy}^i(t) = \int_0^1 \int_0^1 y^2 f_i(x, y, t)\mathrm{d}x\mathrm{d}y = \frac{1}{3} + \frac{1 - e^{-2t}}{4\pi^2},$$
$$\mu_{xy}^i(t) = \int_0^1 \int_0^1 xy f_i(x, y, t)\mathrm{d}x\mathrm{d}y = \frac{1}{4}.$$

In the numerical test, the points approximation of the initial distribution is performed by a transformation of an uniform distribution; the time step used was $\Delta t = 0.01$ and the computations were performed with $N = 100$ particles up to time $T = 5$ (before the moments approaches equilibrium). The relative error $\mathcal{E}_j^i$ between the the analytical moment $\mu_j^i(t)$ and the numerical j-moment $\widetilde{\mu}_j^i(t)$ of the i-solution, is measured by the normalized l^2 norms, which is defined as

$$\mathcal{E}_j^i = \frac{\|\mu_j^i(t) - \widetilde{\mu}_j^i(t)\|^2}{\|\mu_j^i(t)\|^2},$$

for $i = 1, 2$ and $j \in \{x, y, x^2, y^2, xy\}$.

Results are shown in Figs. 1 and 2 for f_1 and f_2 respectively. The x-moments graphs have been omitted from those figures, as the relative error is of the order 10^{-14} and the two curves cannot be distinguished. In Fig. 1, we present the graphs of the moments of the exact solution f_1 (continuous line) and of the numerical solution (dashed lines) vs. time for the first and second moments. In the left-up panel, we compare the graphs for the y-moment and in the right-up panel the graphs of the xy-moment. As these panels show, the numerical and the analytical moments are in a good agreement; lines are very similar and differences are negligible. The left-down panel and the right-down panel of Fig. 1 show the graphs of the x^2-moment and y^2-moment respectively. It is obvious that for the square moments, the agreement is quite reasonable; the relative errors $\mathcal{E}_{xx}^1$ and $\mathcal{E}_{yy}^1$ between the exact and the numerical moments, is of the order 10^{-2}. In Table 1, we report the computed errors, in the l^2-norm, of the first and second moments of the numerical solution f_1.

In Fig. 2 we present the graphs of the moments for f_2. As the figure shows, the qualitative behavior of the moments is similar to the f_1 case; the square and the mixed moments are in a good agreement, the square moments present a greater error. In Table 2 we report the errors, in the l^2-norm, of the first and second moments of the numerical solution f_2.

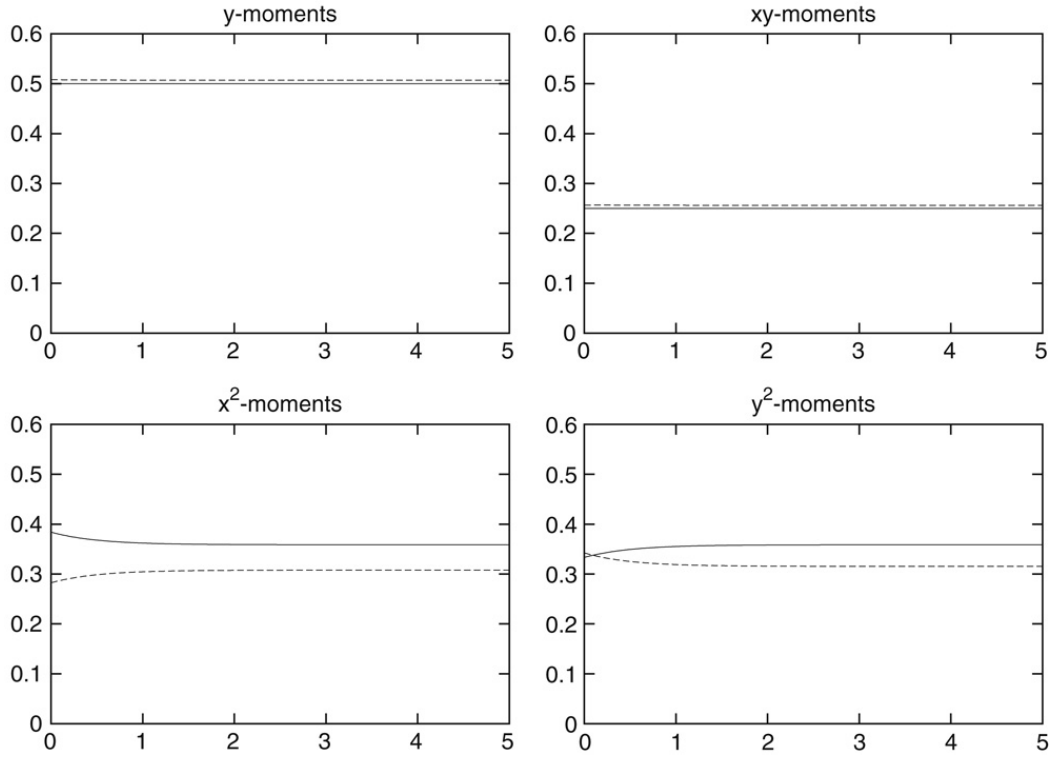

Fig. 1. Moments of the function f_1.

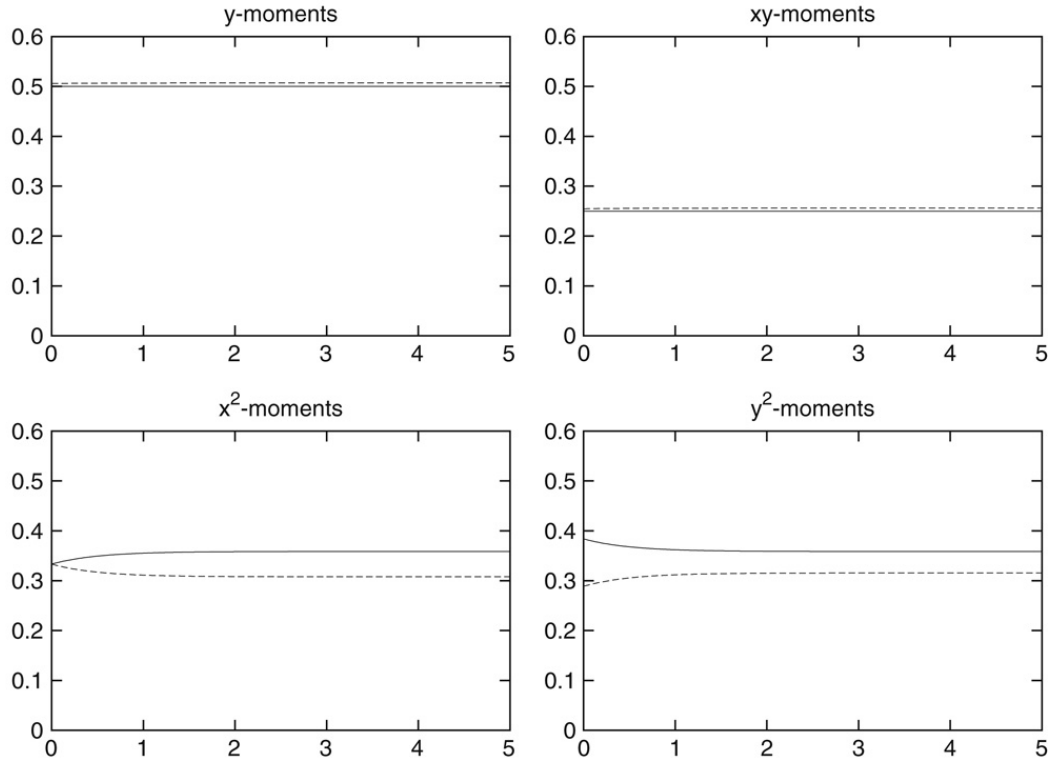

Fig. 2. Moments of the function f_2.

5. Conclusions

We have presented the extension of the MWF method to a Kinetic equation system. Numerical results show that the method is highly accurate, but crucially depends, as all deterministic particle methods, on an accurate point approximation of the initial distribution. The method allows the *approximation nodes*, i.e. the particles, to move in the velocity space,

Table 2
Errors in the l^2-norm for f_2 numerical moments

Error	f_2
$\mathcal{E}_x^1$	6.70×10^{-14}
$\mathcal{E}_y^1$	1.88×10^{-4}
$\mathcal{E}_{xx}^1$	1.73×10^{-2}
$\mathcal{E}_{yy}^1$	1.88×10^{-2}
$\mathcal{E}_{xy}^1$	5.56×10^{-4}

the method is naturally meshfree. As far as linear kernel are concerned, coding the method is rather simple, even if its mathematical description looks hard. Taking into account the properties of integrals with δ functions the computation of the Ψ_i term (12) reduces, for each component, to the computation of the integral of a Heaviside step functions in the given interval. The method does not need to introduce a *mollifier* for treating δ functions.

Even if our test of numerical vs exact solution is very good, this does not substitute a formal convergence proof of the method. This is under investigation and results will be published in due course.

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